LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112318\
Data File : BF110947.D
Acq On : 23 Nov 2018 16:40
Operator : JU/SJ
Sample : J5999-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SSSI-1115-S-AB-1

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.222	18	23	31	rVB	68665	104530	7.77%	0.827%
2	5.175	522	525	540	rBV	33712	53211	3.96%	0.421%
3	5.557	586	590	609	rBV	1024352	1223233	90.94%	9.683%
4	6.563	757	761	781	rBV	1236995	1345077	100.00%	10.648%
5	6.704	781	785	793	rVV	1553715	1311724	97.52%	10.384%
6	6.934	821	824	833	rBV	388704	345654	25.70%	2.736%
7	7.087	847	850	866	rBV	935445	870039	64.68%	6.887%
8	7.498	917	920	939	rBV	667418	816635	60.71%	6.465%
9	8.216	1039	1042	1063	rBV	373949	457916	34.04%	3.625%
10	9.286	1221	1224	1234	rBV	1049388	994268	73.92%	7.871%
11	9.686	1289	1292	1298	rVB	62258	60293	4.48%	0.477%
12	9.975	1338	1341	1351	rVB	451288	472439	35.12%	3.740%
13	10.775	1473	1477	1488	rBV	586385	665924	49.51%	5.272%
14	11.475	1592	1596	1599	rBV	427645	398392	29.62%	3.154%
15	11.498	1599	1600	1607	rVB	58177	44224	3.29%	0.350%
16	11.975	1677	1681	1685	rBV2	88138	93991	6.99%	0.744%
17	12.010	1685	1687	1693	rVB	17084	18390	1.37%	0.146%
18	12.092	1698	1701	1704	rBV2	16317	17923	1.33%	0.142%
19	12.692	1800	1803	1808	rBV	126025	127880	9.51%	1.012%
20	12.757	1812	1814	1817	rBV2	39326	34710	2.58%	0.275%
21	12.927	1840	1843	1849	rVB	129977	121021	9.00%	0.958%
22	13.051	1861	1864	1868	rBV	914426	781692	58.12%	6.188%
23	13.145	1877	1880	1885	rVB3	12172	15934	1.18%	0.126%
24	13.257	1891	1899	1903	rBV	32906	66974	4.98%	0.530%
25	13.321	1907	1910	1913	rVV2	15367	17738	1.32%	0.140%
26	13.363	1914	1917	1923	rVB2	16297	19968	1.48%	0.158%
27	13.457	1930	1933	1936	rBV2	14315	23096	1.72%	0.183%
28	13.592	1954	1956	1960	rBV2	17156	19499	1.45%	0.154%
29	13.927	2010	2013	2019	rBV3	60618	76927	5.72%	0.609%
30	14.127	2042	2047	2050	rBV2	443144	499333	37.12%	3.953%
31	14.151	2050	2051	2056	rVB	75766	66976	4.98%	0.530%
32	14.239	2064	2066	2070	rVB	31456	29934	2.23%	0.237%
33	14.292	2073	2075	2081	rVB4	17242	20508	1.52%	0.162%
34	14.516	2111	2113	2115	rBV	19438	15132	1.12%	0.120%

LSC Area Percent Report

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Operator : JU/SJ
Sample : J5999-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SSSI-1115-S-AB-1

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.545	2115	2118	2123	rVV2	56040	61809	4.60%	0.489%
36	14.863	2168	2172	2175	rBV	78032	89316	6.64%	0.707%
37	15.210	2227	2231	2242	rVB	148921	252641	18.78%	2.000%
38	15.527	2282	2285	2290	rBV2	31670	53236	3.96%	0.421%
39	15.604	2293	2298	2303	rVB2	129404	186712	13.88%	1.478%
40	15.657	2303	2307	2313	rBV	238938	331963	24.68%	2.628%
41	16.057	2370	2375	2380	rVB	88044	149654	11.13%	1.185%
42	16.339	2419	2423	2432	rVB5	47274	94807	7.05%	0.751%
43	16.580	2460	2464	2471	rVB	41896	63654	4.73%	0.504%
44	16.798	2497	2501	2511	rVB6	38675	78840	5.86%	0.624%
45	17.398	2600	2603	2610	rVB6	22068	38386	2.85%	0.304%

Sum of corrected areas: 12632203

LSC Report - Integrated Chromatogram

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Sample : J5999-05
Misc :
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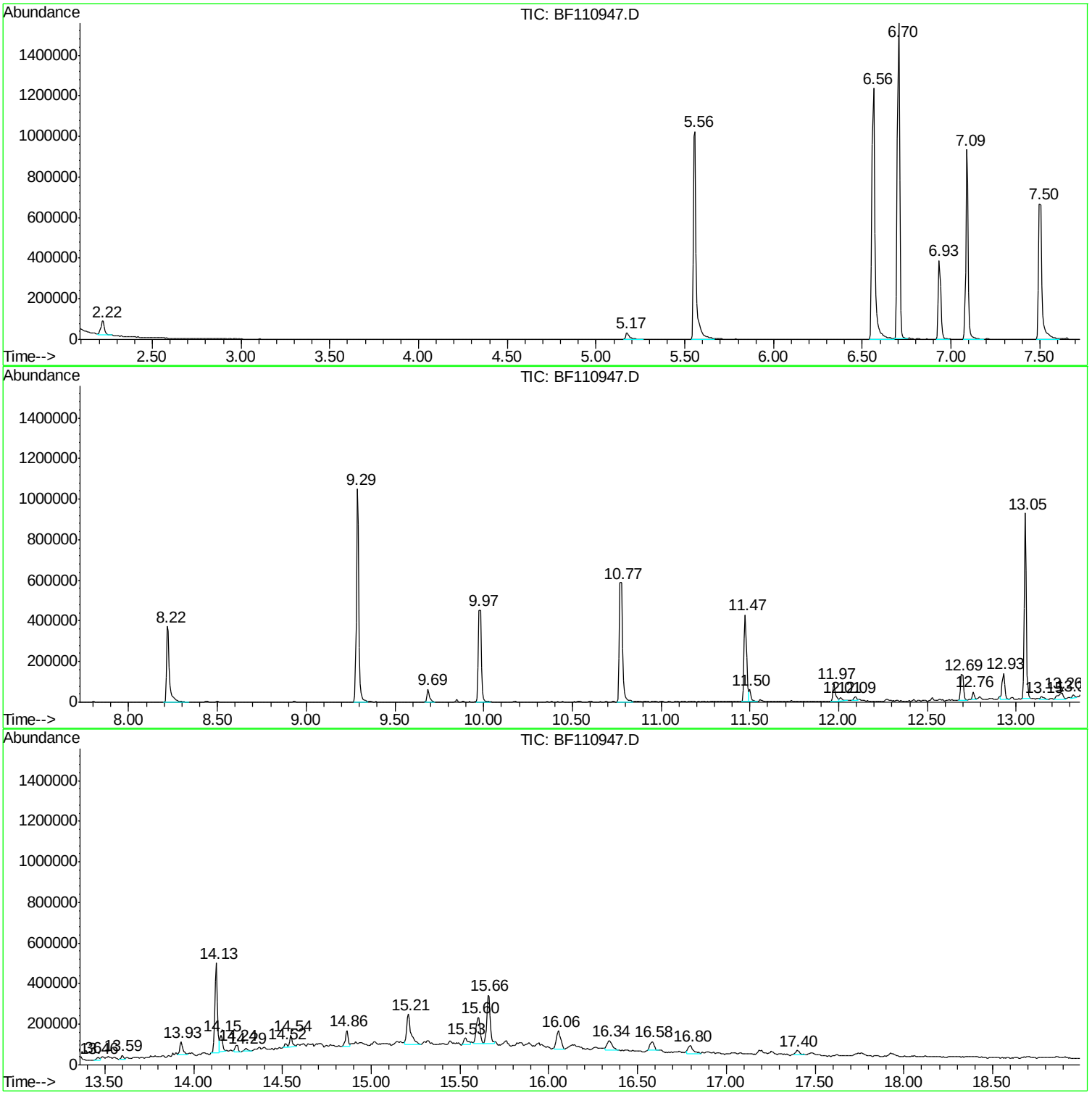
Instrument : BNA_F
ClientSampleId : SSSI-1115-S-AB-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112318\
Data File : BF110947.D
Acq On : 23 Nov 2018 16:40
Operator : JU/SJ
Sample : J5999-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SSSI-1115-S-AB-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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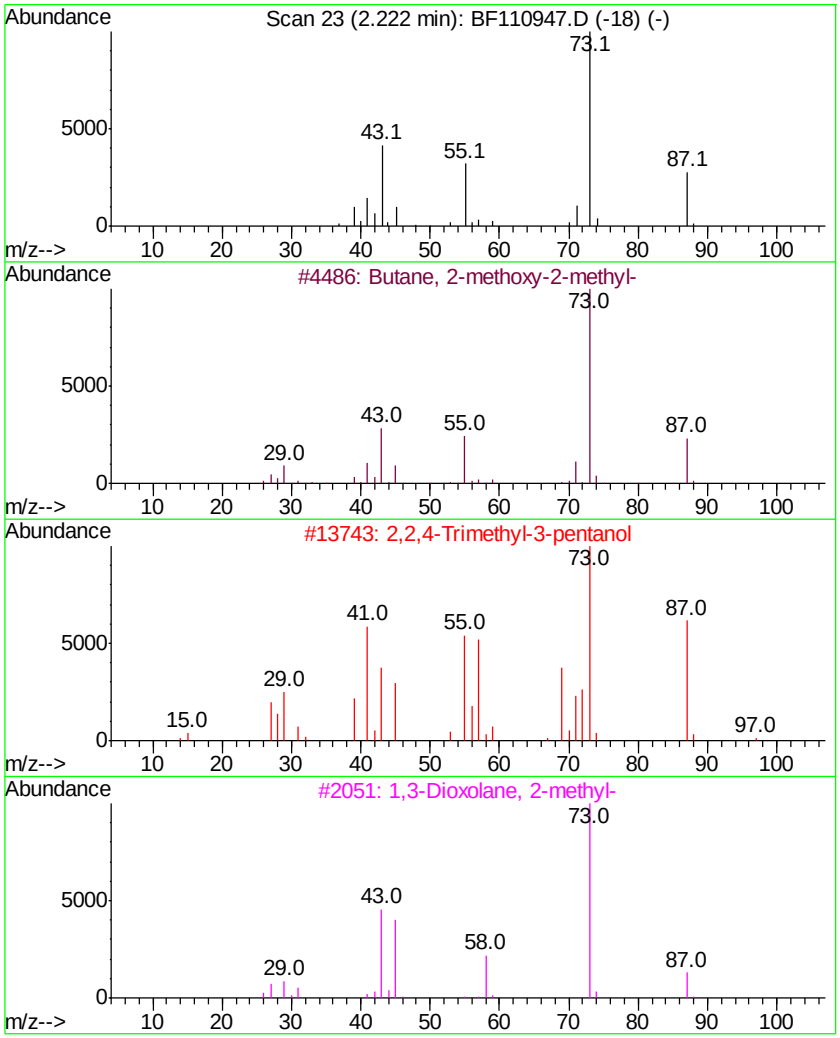
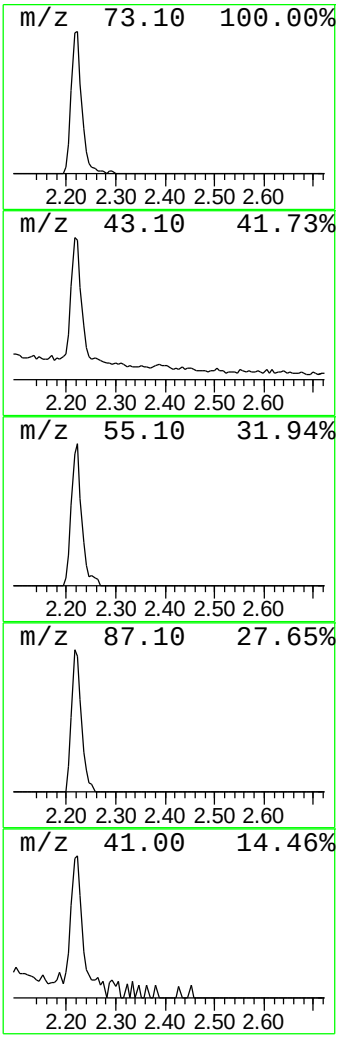
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.22	6.05 ng	104530	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	17
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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Operator : JU/SJ
Sample : J5999-05
Misc :
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Instrument : BNA_F
ClientSampleId : SSSI-1115-S-AB-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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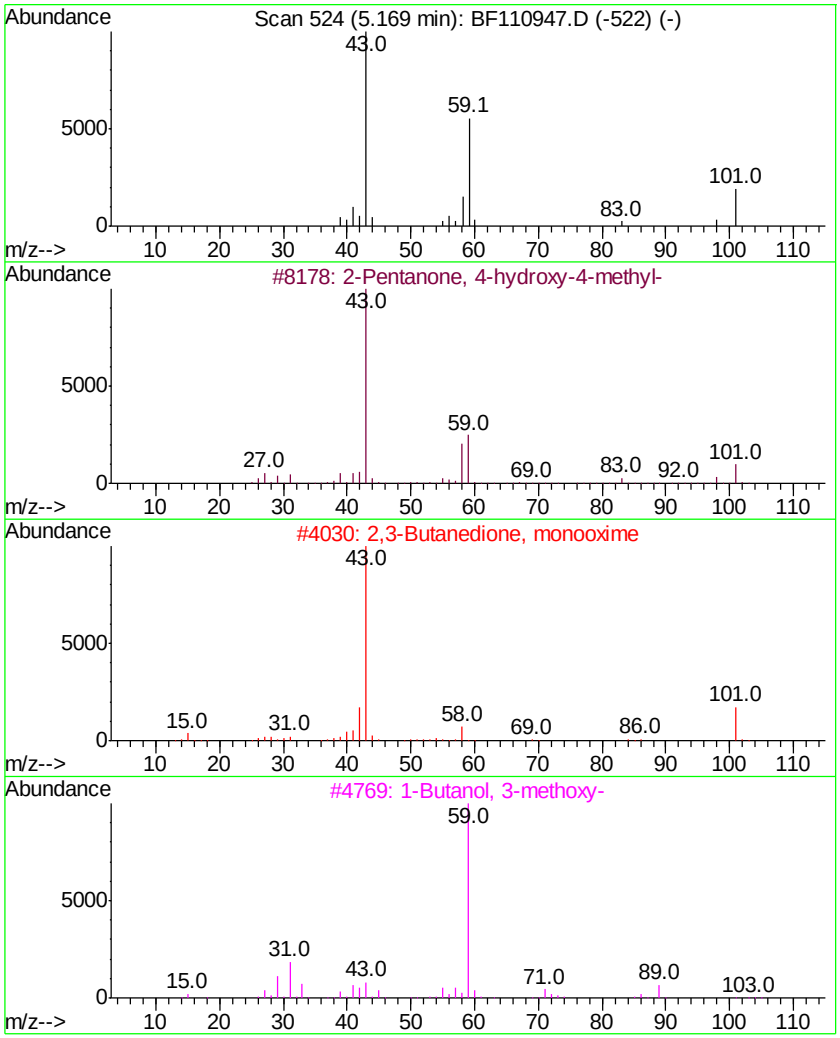
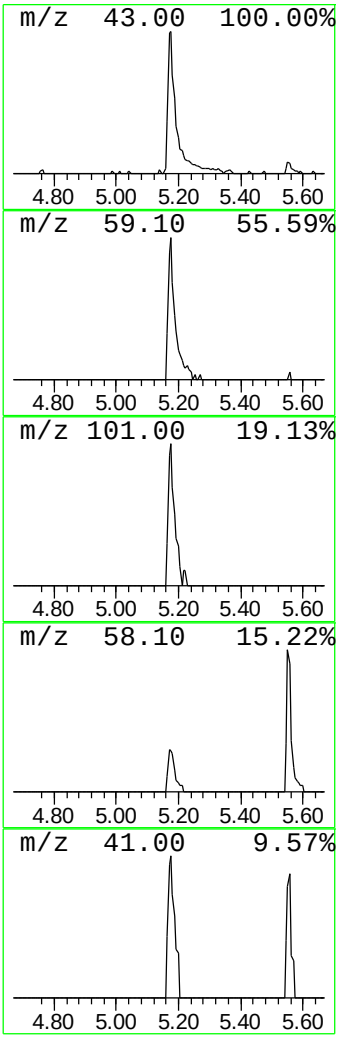
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	3.08 ng	53211	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3	1-Butanol, 3-methoxy-	104	C5H12O2	002517-43-3	9
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112318\
Data File : BF110947.D
Acq On : 23 Nov 2018 16:40
Operator : JU/SJ
Sample : J5999-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SSSI-1115-S-AB-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

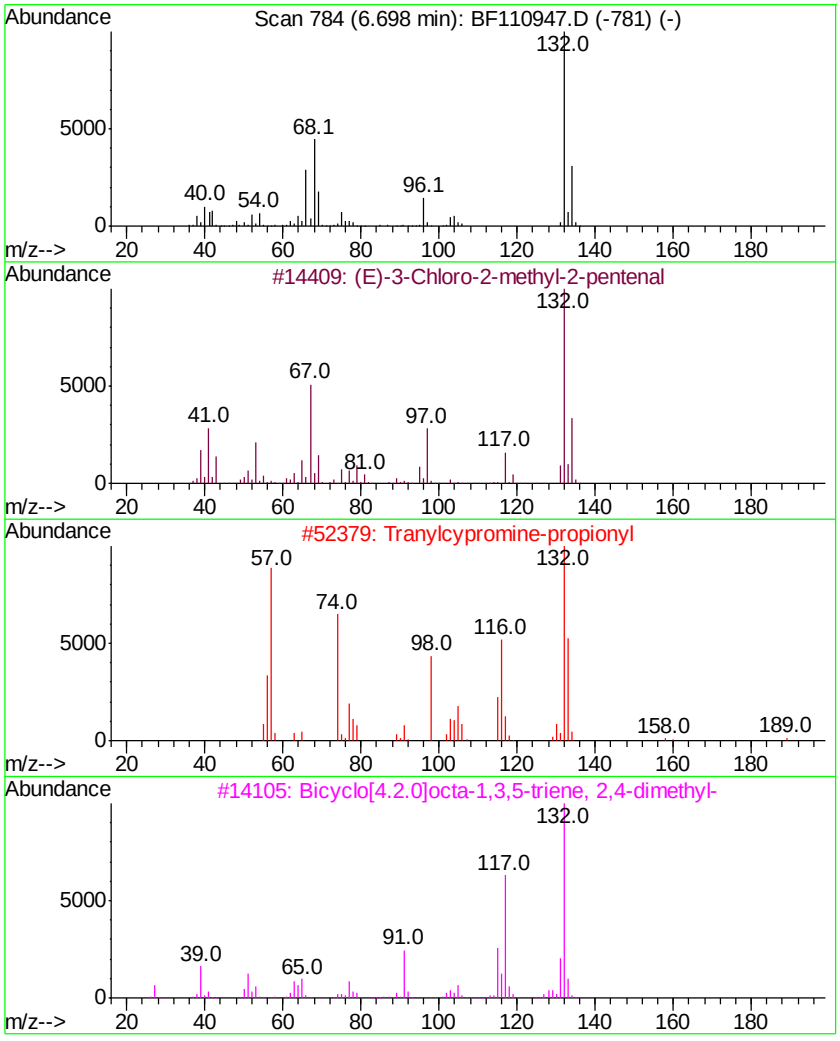
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

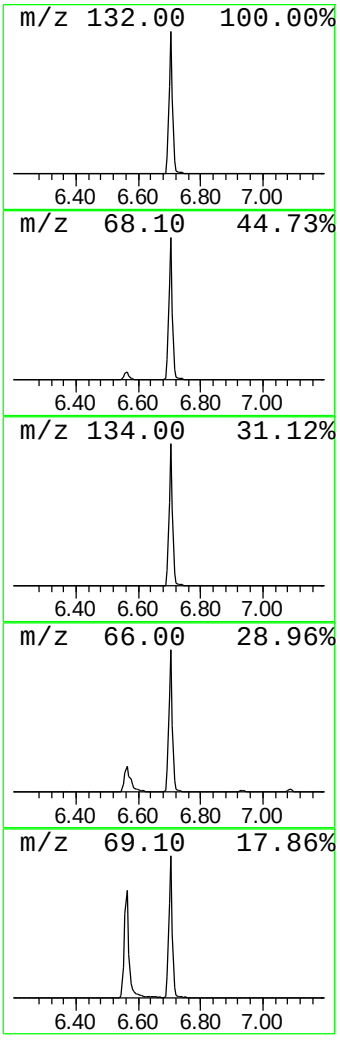
****

Peak Number 3 unknown6.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	75.90 ng	1311720	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





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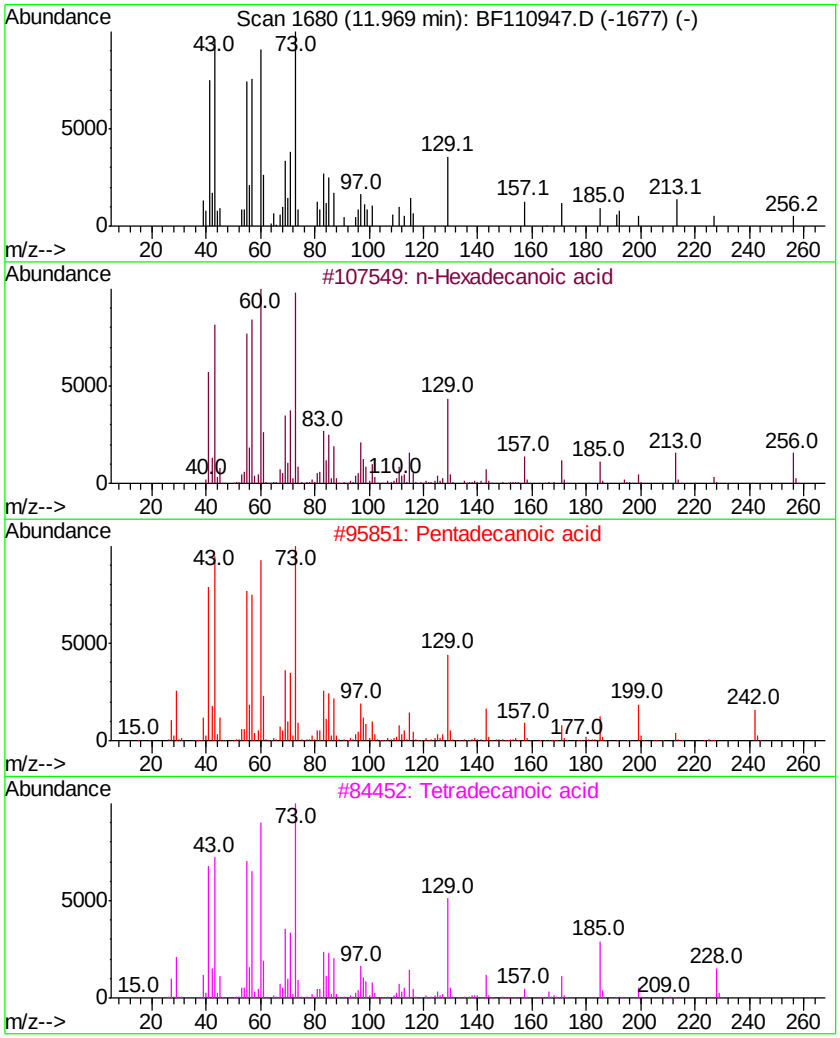
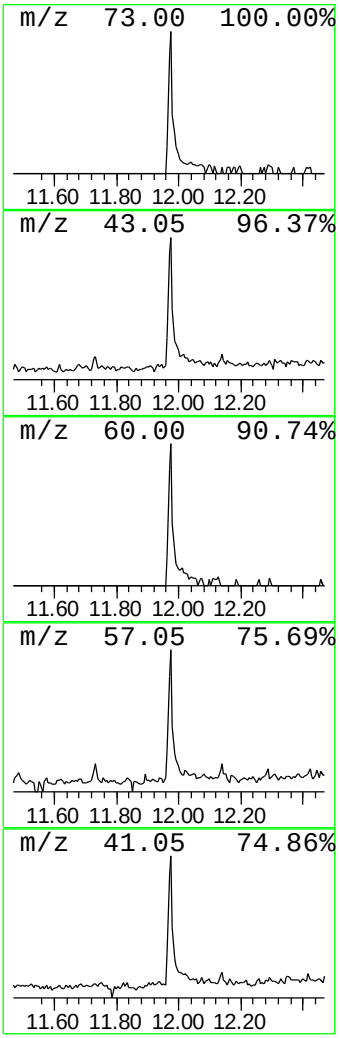
Peak Number 5 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.97	4.72 ng	93991	Phenanthrene-d10	11.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	52





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Misc :
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Instrument : BNA_F
ClientSampleId : SSSI-1115-S-AB-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
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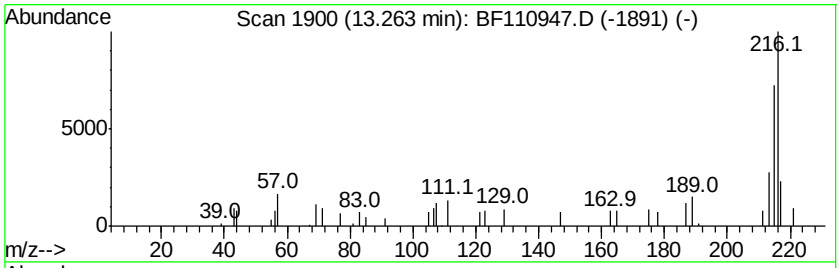
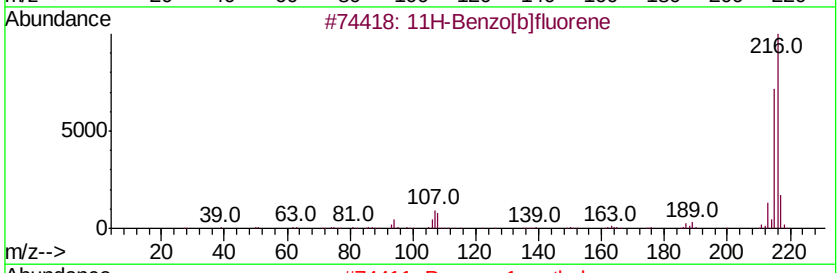
****

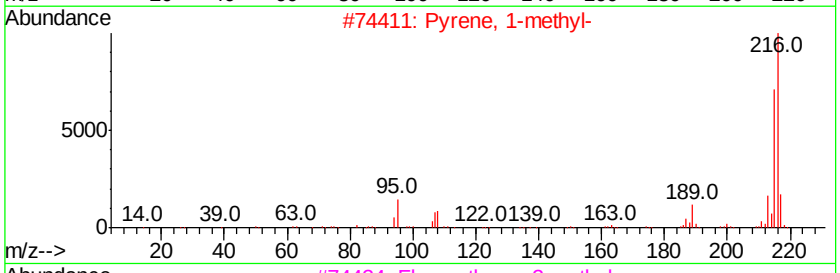
Peak Number 6 11H-Benzo[b]fluorene Concentration Rank 13

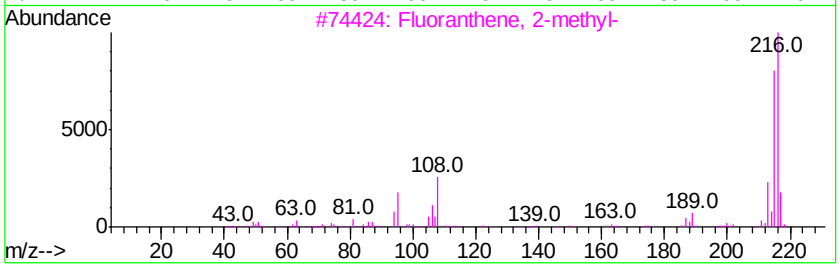
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.26	2.68 ng	66974	Chrysene-d12	14.13

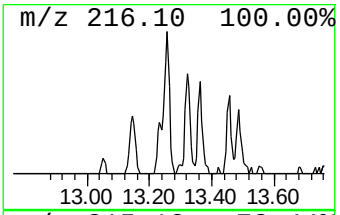
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	94
2	Pyrene, 1-methyl-	216	C17H12	002381-21-7	94
3	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	87
4	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	72
5	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	72

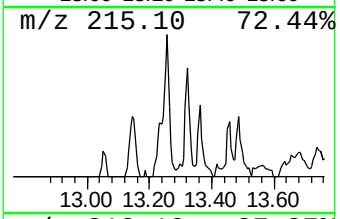


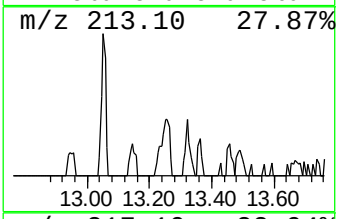


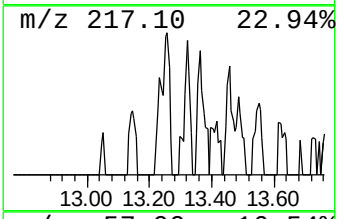


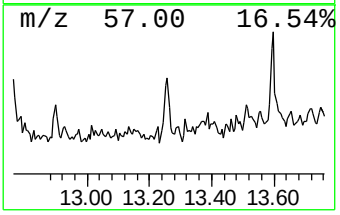












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Instrument : BNA_F
ClientSampleId : SSSI-1115-S-AB-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

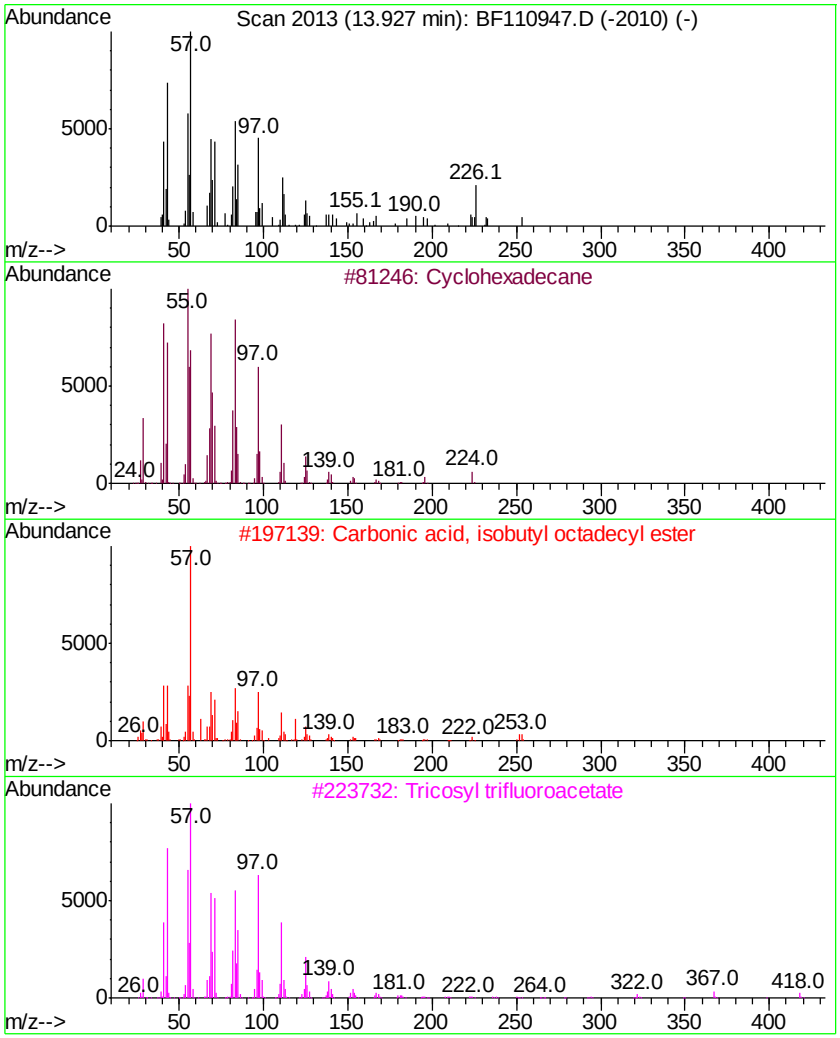
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

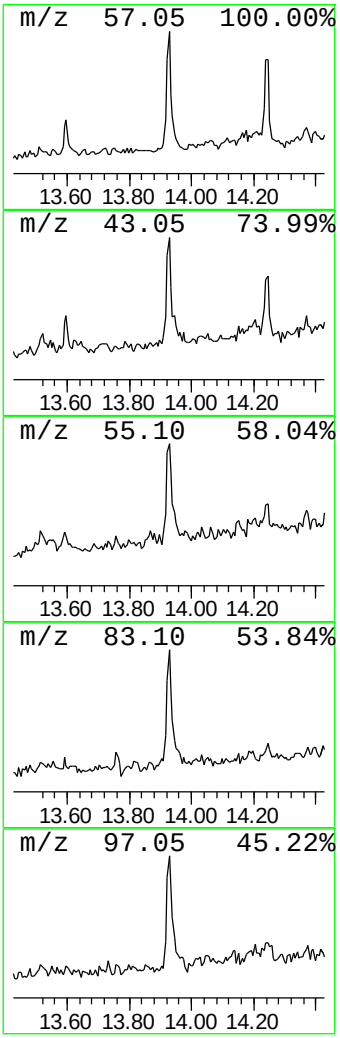
****

Peak Number 7 Cyclohexadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.93	3.08 ng	76927	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	86
2	Carbonic acid, isobutyl octadecy...	370	C23H46O3	1000314-61-5	83
3	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	74
4	Cyclopentane, (4-octyldodecyl)-	350	C25H50	005638-09-5	74
5	Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	74





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112318\
Data File : BF110947.D
Acq On : 23 Nov 2018 16:40
Operator : JU/SJ
Sample : J5999-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SSSI-1115-S-AB-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

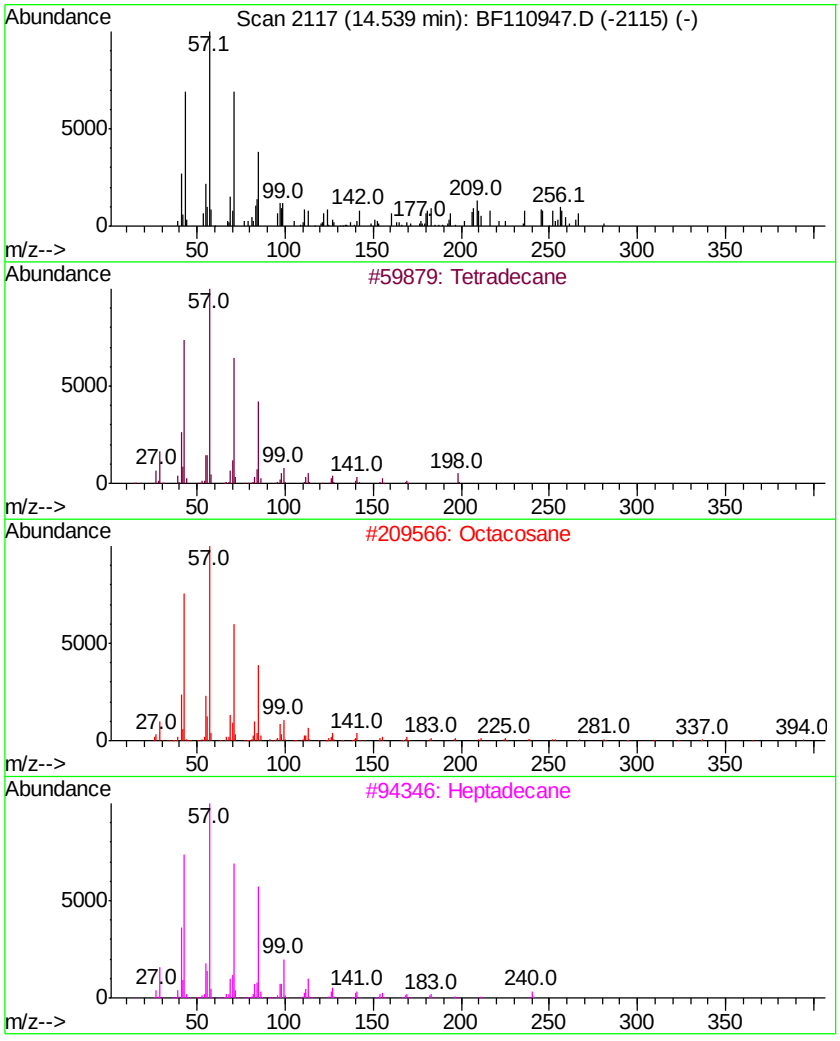
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

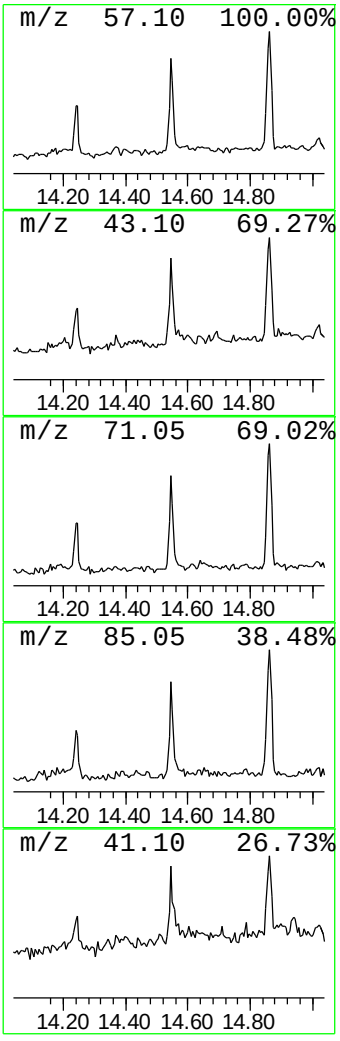
****

Peak Number 8 Tetradecane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.54	2.48 ng	61809	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	94
2	Octacosane	394	C28H58	000630-02-4	81
3	Heptadecane	240	C17H36	000629-78-7	81
4	Octadecane, 2-methyl-	268	C19H40	001560-88-9	80
5	Hexacosane	366	C26H54	000630-01-3	74





Library Search Compound Report

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Data File : BF110947.D
Acq On : 23 Nov 2018 16:40
Operator : JU/SJ
Sample : J5999-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SSSI-1115-S-AB-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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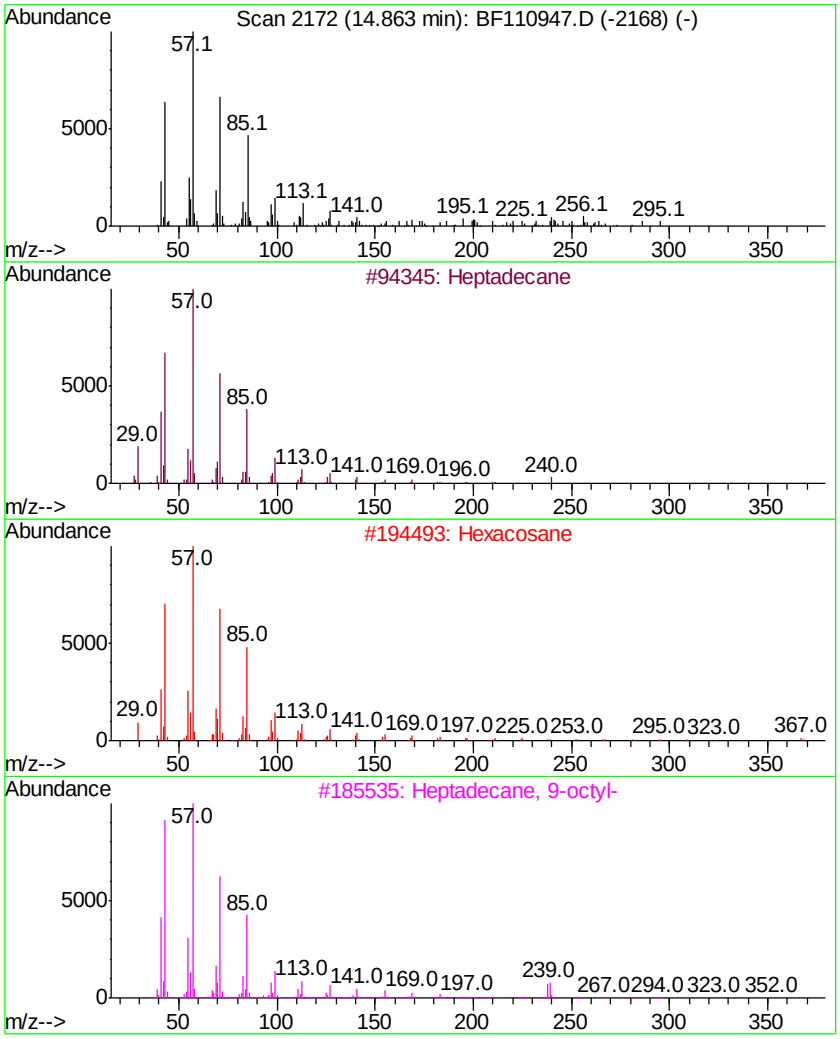
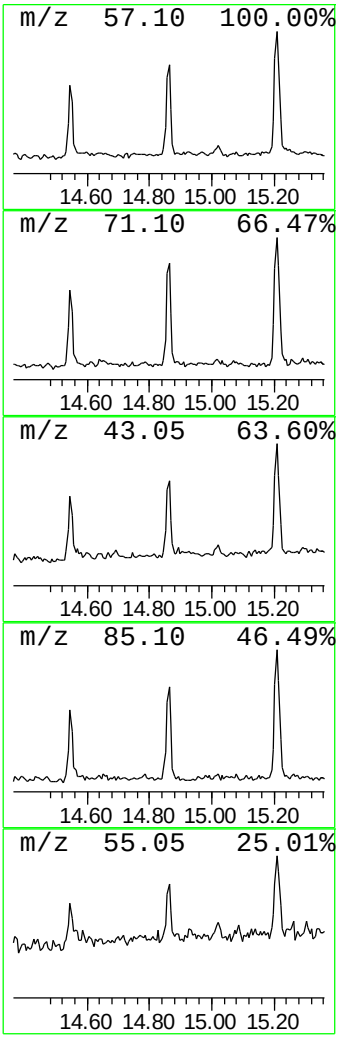
Peak Number 9 Heptadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.86	3.58 ng	89316	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	93
2	Hexacosane	366	C26H54	000630-01-3	90
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
4	Tetracosane	338	C24H50	000646-31-1	87
5	Tetratetracontane	619	C44H90	007098-22-8	87





Library Search Compound Report

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Data File : BF110947.D
Acq On : 23 Nov 2018 16:40
Operator : JU/SJ
Sample : J5999-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SSSI-1115-S-AB-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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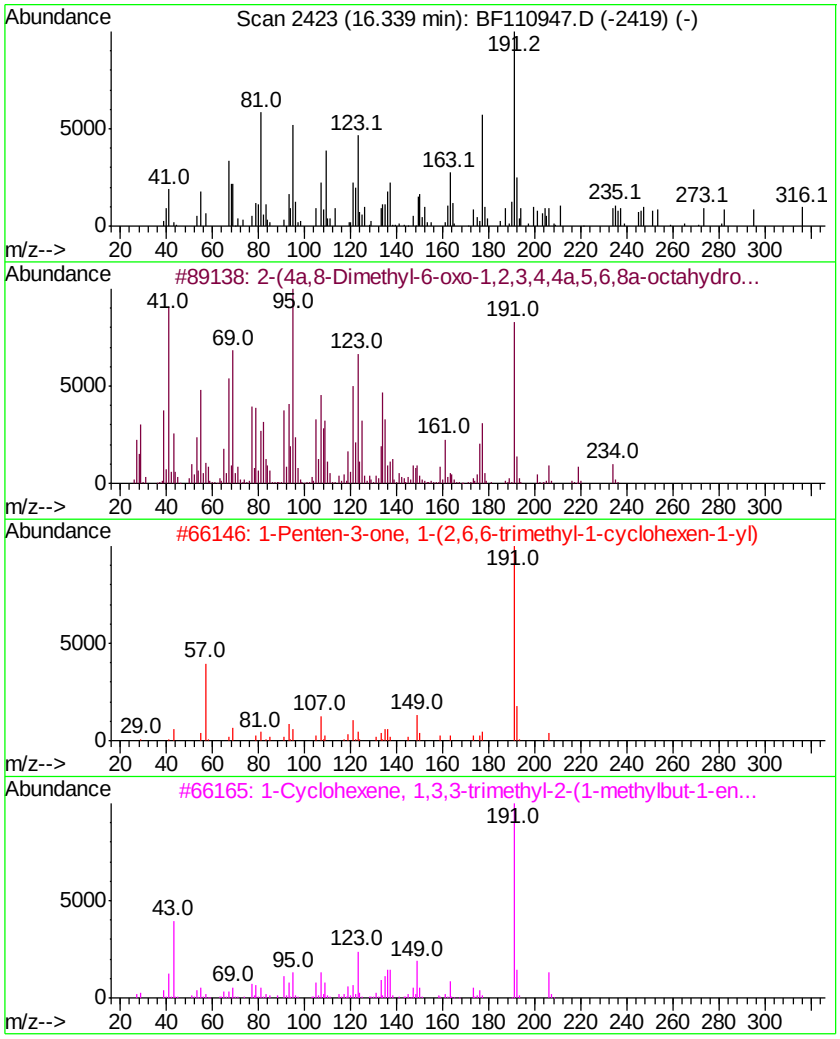
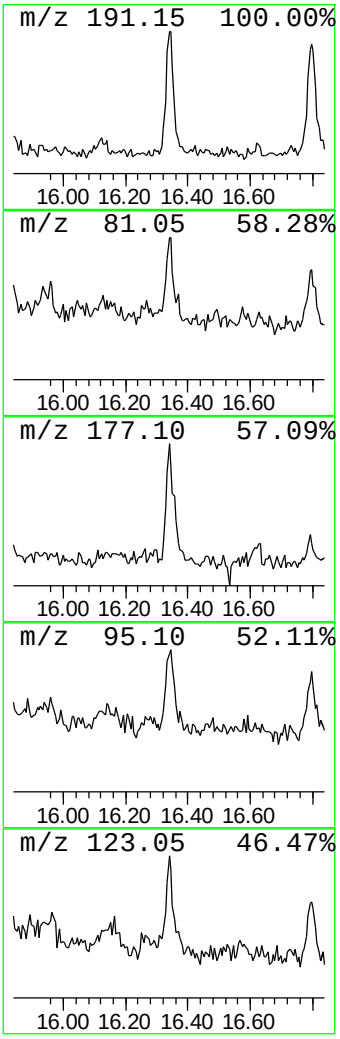
Peak Number 12 unknown16.34 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.34	5.71 ng	94807	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(4a,8-Dimethyl-6-oxo-1,2,3,4,4...	234	C15H22O2	1000190-21-8	35
2	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	27
3	1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	25
4	3,7-Diisopropyl-5-methyl-1,2(4H)...	192	C12H20N2	088829-71-4	25
5	Pyrrolidine, 1-(9-borabicyclo[3....	191	C12H22BN	022516-41-2	22





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Acq On : 23 Nov 2018 16:40
Operator : JU/SJ
Sample : J5999-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SSSI-1115-S-AB-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
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TIC Integration Parameters: LSCINT.P

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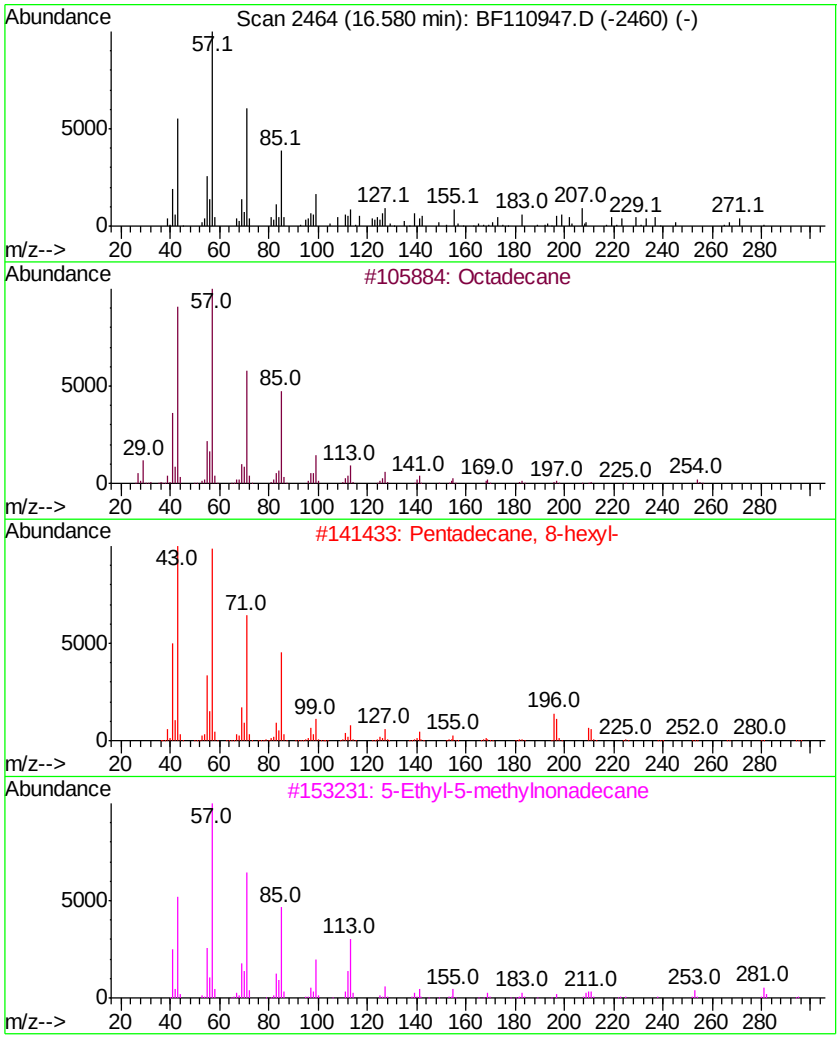
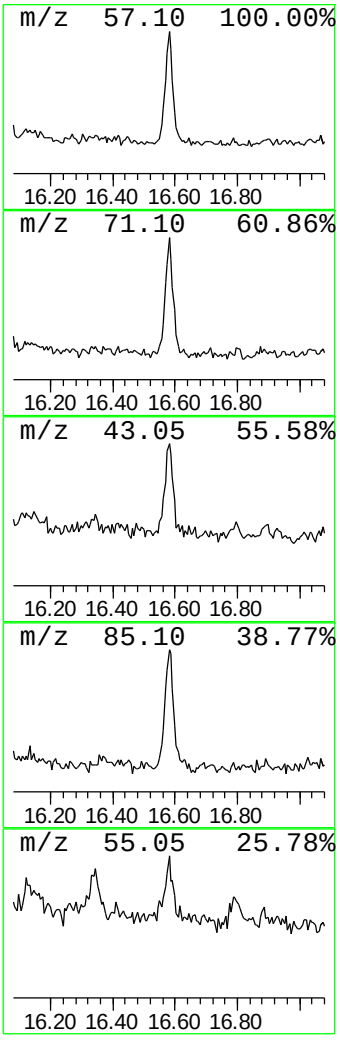
Peak Number 13 Octadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.58	3.84 ng	63654	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	72
2	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	72
3	5-Ethyl-5-methylnonadecane	310	C22H46	1000360-42-7	72
4	Hexacosane	366	C26H54	000630-01-3	72
5	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	72





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112318\
Data File : BF110947.D
Acq On : 23 Nov 2018 16:40
Operator : JU/SJ
Sample : J5999-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SSSI-1115-S-AB-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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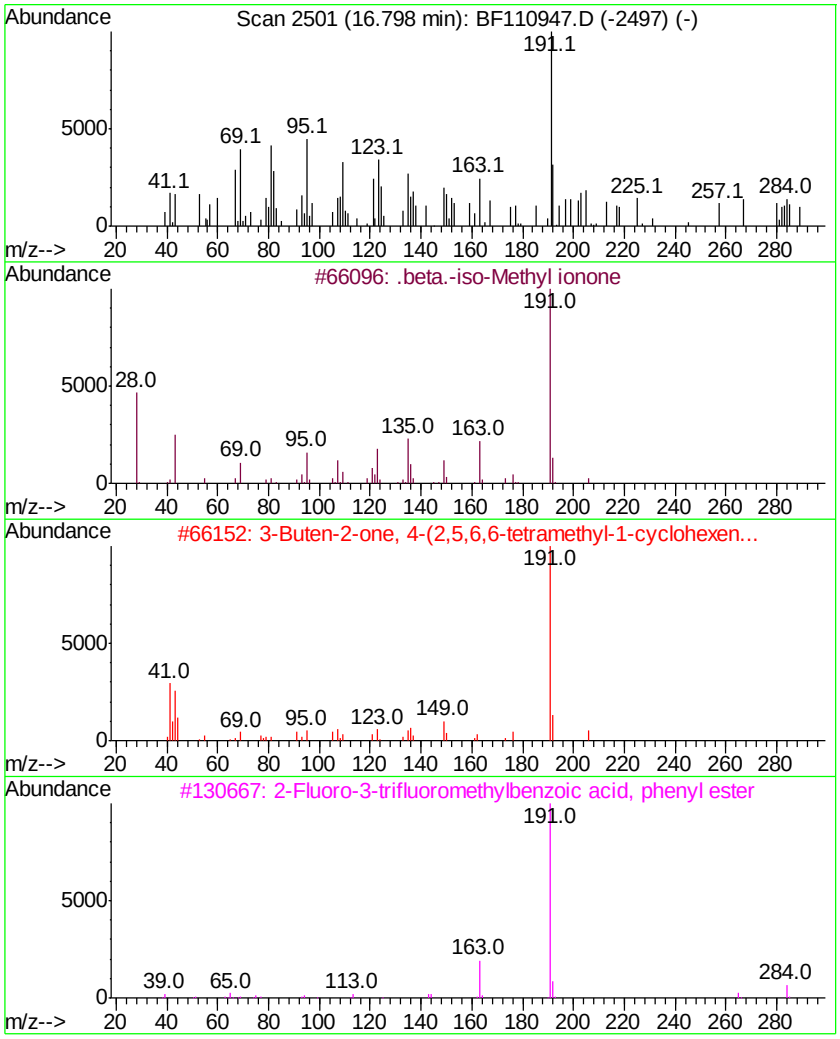
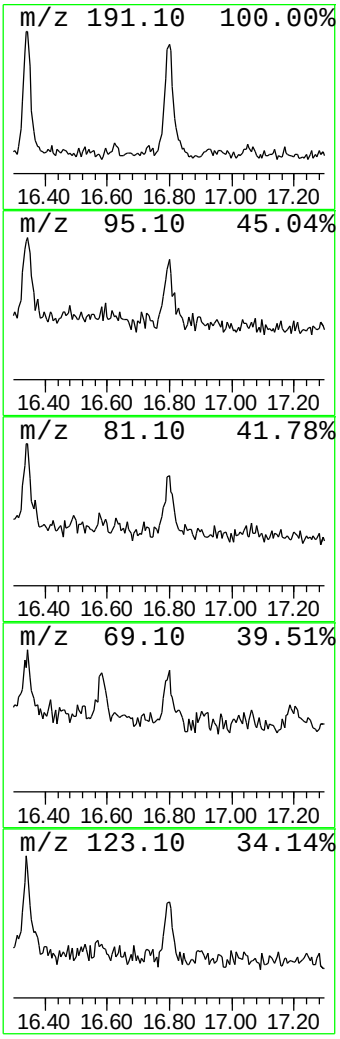
Peak Number 14 unknown16.80 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.80	4.75 ng	78840	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	42
2	3-Buten-2-one, 4-(2,5,6,6-tetram...	206	C14H22O	000079-70-9	38
3	2-Fluoro-3-trifluoromethylbenzoi...	284	C14H8F4O2	1000357-64-3	38
4	3-Fluoro-4-trifluoromethylbenzoi...	284	C14H8F4O2	1000357-93-7	38
5	Anthracene, 9-dodecyltetradecahy...	360	C26H48	055401-75-7	37





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Data File : BF110947.D
Acq On : 23 Nov 2018 16:40
Operator : JU/SJ
Sample : J5999-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SSSI-1115-S-AB-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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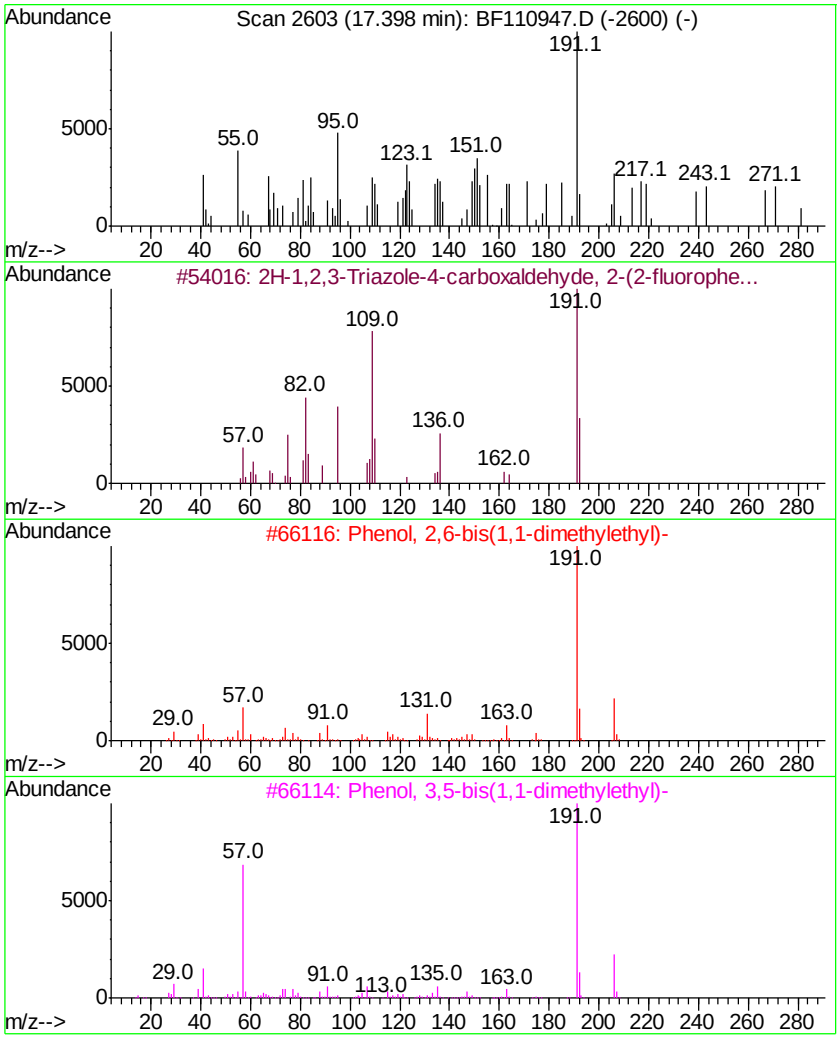
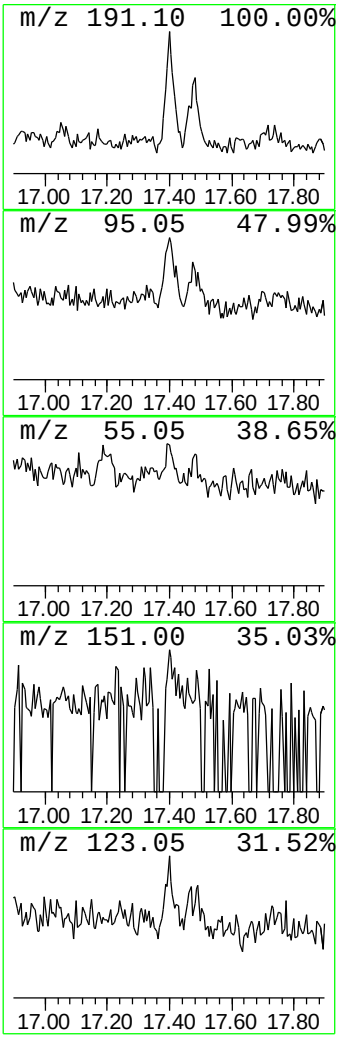
Peak Number 15 unknown17.40 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.40	2.31 ng	38386	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-1,2,3-Triazole-4-carboxaldehy...	191	C9H6FN3O	051306-43-5	35
2	Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	27
3	Phenol, 3,5-bis(1,1-dimethylethyl)-	206	C14H22O	001138-52-9	27
4	1-(3,6,6-Trimethyl-1,6,7,7a-tetr...	206	C13H18O2	1000194-97-2	27
5	Phenol, 2,5-bis(1,1-dimethylethyl)-	206	C14H22O	005875-45-6	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF112318\
Data File : BF110947.D
Acq On : 23 Nov 2018 16:40
Operator : JU/SJ
Sample : J5999-05
Misc :
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Instrument : BNA_F
ClientSampleId : SSSI-1115-S-AB-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	2.22	6.0	ng	104530	1	6.93	345654	20.0
2-Pentanone, 4-hy...	5.17	3.1	ng	53211	1	6.93	345654	20.0
unknown6.70	6.70	75.9	ng	1311720	1	6.93	345654	20.0
n-Hexadecanoic acid	11.97	4.7	ng	93991	4	11.47	398392	20.0
11H-Benzo[b]fluorene	13.26	2.7	ng	66974	5	14.13	499333	20.0
Cyclohexadecane	13.93	3.1	ng	76927	5	14.13	499333	20.0
Tetradecane	14.54	2.5	ng	61809	5	14.13	499333	20.0
Heptadecane	14.86	3.6	ng	89316	5	14.13	499333	20.0
unknown16.34	16.34	5.7	ng	94807	6	15.66	331963	20.0
Octadecane	16.58	3.8	ng	63654	6	15.66	331963	20.0
unknown16.80	16.80	4.8	ng	78840	6	15.66	331963	20.0
unknown17.40	17.40	2.3	ng	38386	6	15.66	331963	20.0